

Supporting Information

Appraisal of Novel Azomethine-Thioxoimidazolidinone conjugates as ecto-5'- nucleotidase inhibitors: Synthesis and Molecular Docking Studies

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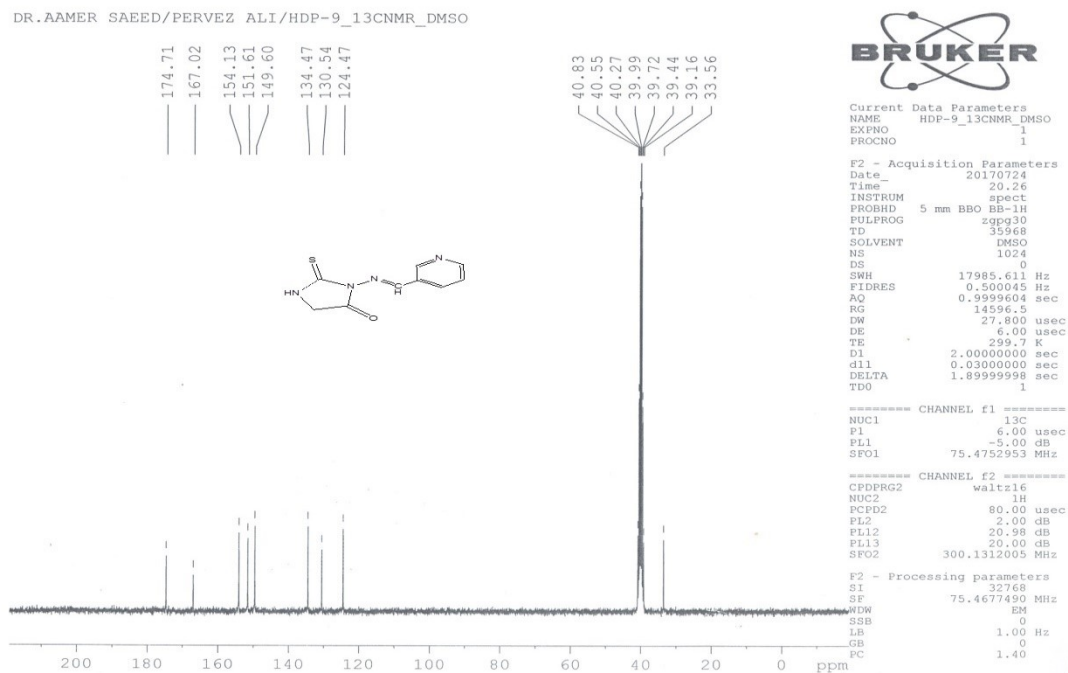
† Both these authors contributed equally

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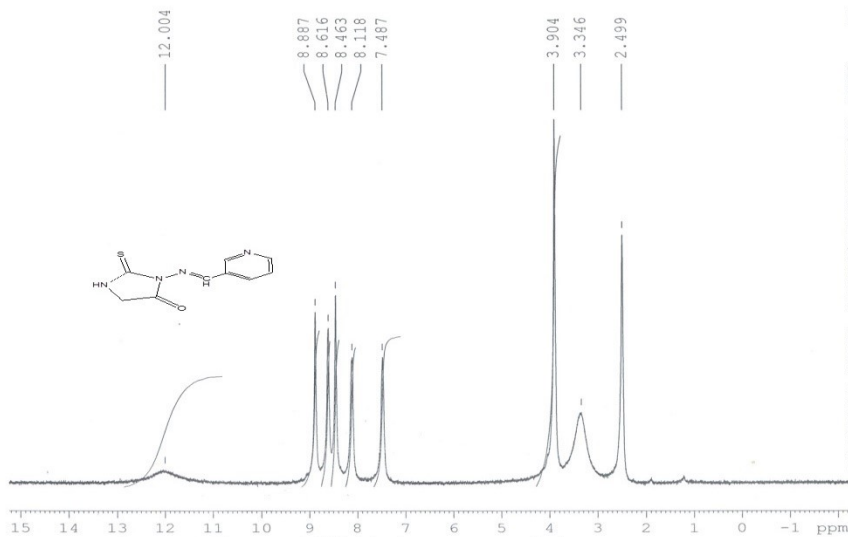
Prof. Dr. Jamshed Iqbal; drjamshed@cuiatd.edu.pk

Supplementary



(E)-3-((pyridin-3-ylmethylene)amino)-2-thioxoimidazolidin-4-one¹³CNMR (4h)

DR. AAMER SAEED/PERVEZ ALI/HDP-9_1HNMR_DMSO



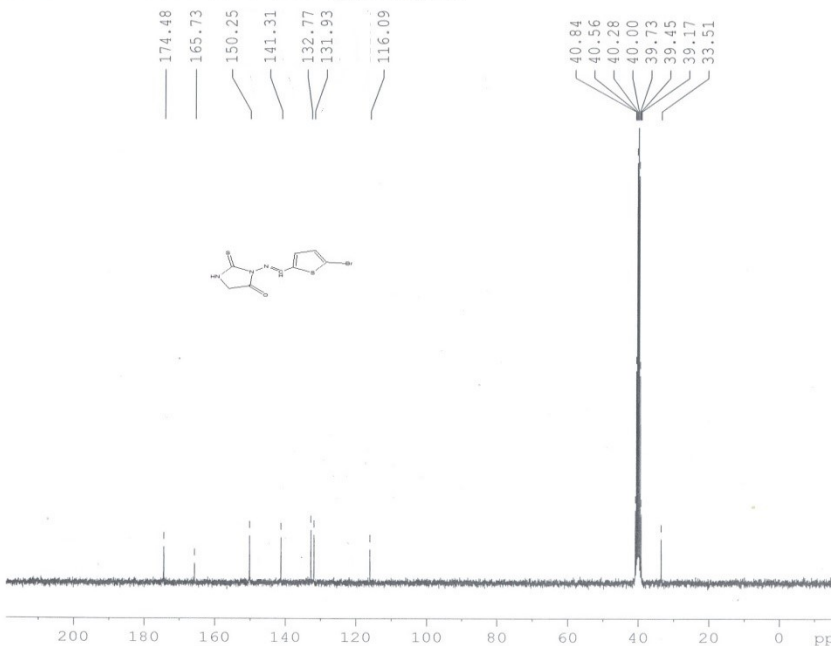
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PROCNO 1

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FIDRES 0.094190 Hz
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F2 - Processing parameters
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SF 300.1297771 MHz
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LB 0.30 Hz
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(E)-3-((pyridin-3-ylmethylene) amino)-2-thioxoimidazolidin-4-one¹HNMR (4h)

DR. AAMER SAEED/PERVEZ ALI/HDP-2_13CNMR_DMSO



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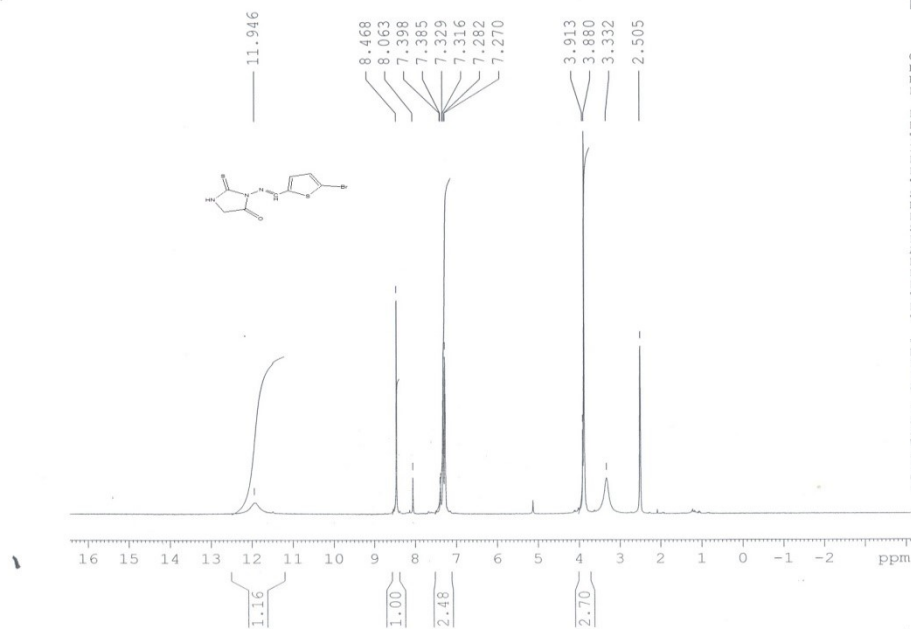
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AQ 0.9999604 sec
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TE 300.8 K
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d11 0.03000000 sec
DELTA 1.89999998 sec
TDO 1

CHANNEL f1
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P1 6.00 usec
PL1 -5.00 dB
SFO1 75.4752953 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 20.98 dB
PL13 20.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
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SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

(E)-3-(((5-bromothiophen-2-yl)methylene)amino)-2-thioxoimidazolidin-4-one¹HNMR(4b)

DR.AAMER SAEED/PERVEZ ALI/HDP-2_1HNMR_DMSO



Current Data Parameters
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EXPNO 1
PROCNO 1

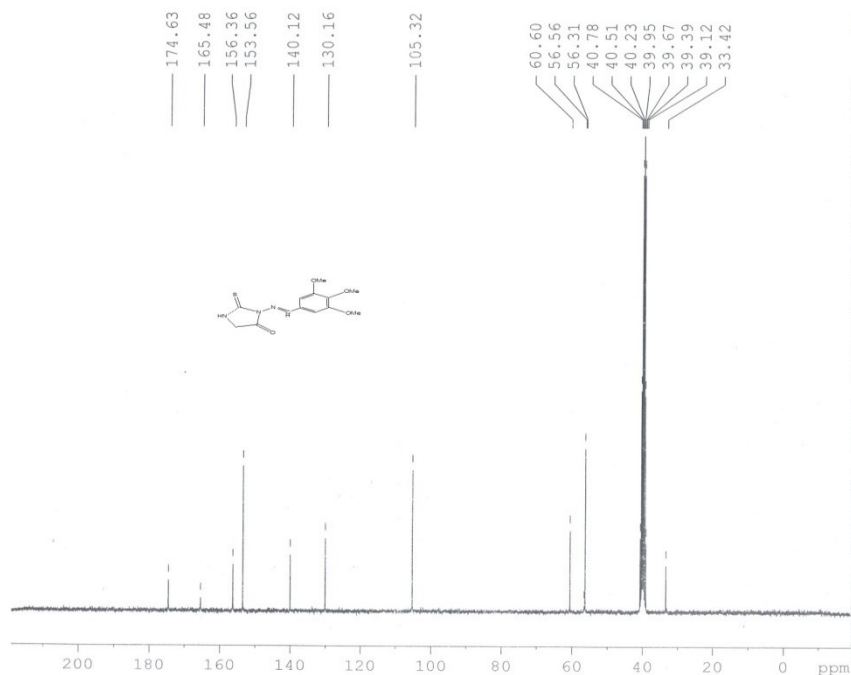
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TD 65536
SOLVENT DMSO
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SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 456.1
DW 81.000 usec
DE 6.00 usec
TE 299.9 K
D1 1.0000000 sec
TDO 1

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P1 9.00 usec
PL1 2.00 dB
SF01 300.1318534 MHz

F2 - Processing parameters
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SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

(E)-3-(((5-bromothiophen-2-yl)methylene)amino)-2-thioxoimidazolidin-4-one¹³CNMR (4b)

DR.AAMER SAEED/PERVEZ ALI/HDP5_13CNMR_DMSO



Current Data Parameters
NAME HDP5_13CNMR_DMSO
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PROCNO 1

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DELTA 1.89999998 sec
TDO 1

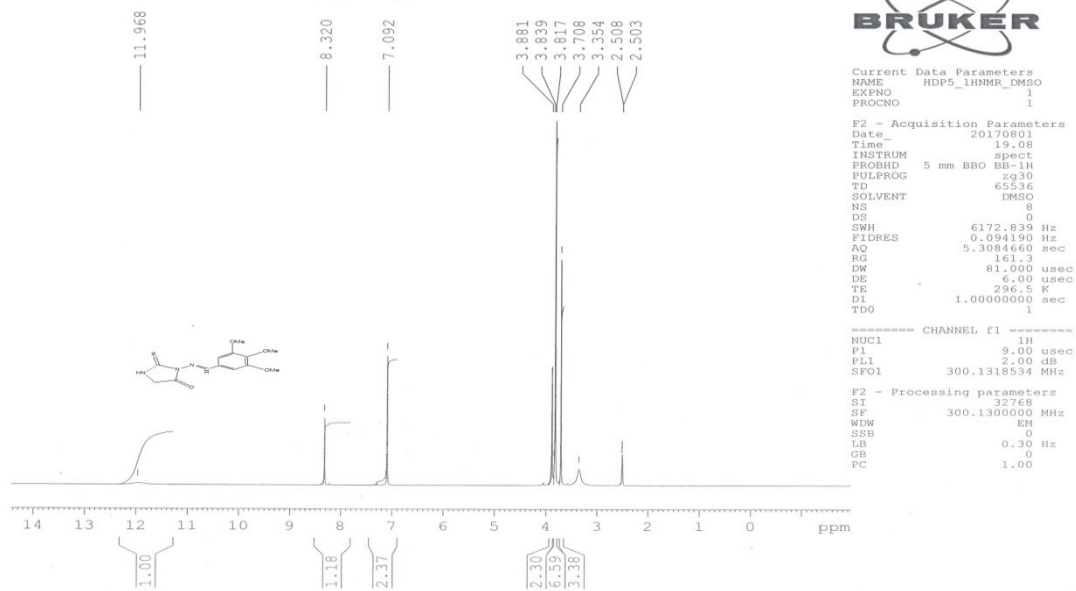
----- CHANNEL f1 -----
NUC1 13C
P1 6.00 usec
PL1 -5.00 dB
SF01 75.4752953 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 20.98 dB
PL13 20.00 dB
SF02 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

(E)-2-thioxo-3-((3,4,5-trimethoxybenzylidene)amino)imidazolidin-4-one¹HNMR (4e)

DR.AAMER SAEED/PERVEZ ALI/HDP5_1HNMR_DMSO



(E)-2-thioxo-3-((3,4,5-trimethoxybenzylidene)amino)imidazolidin-4-one¹³CNMR (4e)